

Redesign of Industrial Apparatus using Multi-Objective Bayesian Optimisation

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1 Introduction

Design optimisation using Computational Fluid Dynamics (CFD) often requires extremising multiple (and often conflicting) objectives simultaneously. For instance, a heat exchanger design will require maximising the heat transfer across the media, while minimising the pressure drop across the apparatus. In such cases, usually there is no unique solution, but a range of solutions trading off between the objectives. The set of solutions optimally trading off the objectives are known as the Pareto set, and in practice only an approximation of the set may be achieved. Multi-Objective Evolutionary Algorithms (MOEAs) are known to perform well in estimating the optimal Pareto set. However, they require thousands of function evaluations, which is impractical with computationally expensive simulations. An alternative is to use Multi-Objective Bayesian Optimisation (MOBO) method that has been proved to be an effective approach with limited budget on function evaluations [1]. In this work, we illustrate a newly developed MOBO framework in [1] with OpenFOAM 2.3.1 to locate a good estimation of the optimal Pareto set for a range of industrial cases.

2 Methodology

MOBO is a model-based global search strategy that sequentially samples the design space at likely locations of the optimal Pareto set solutions. It starts with a filling the design space (e.g. by Latin Hypercube Sampling). The initial set of shapes are then expensively evaluated with appropriate CFD simulations. An aggregation (or scalarisation) function may then be used to combine the multiple objective functions into a single objective function. Here we used hypervolume (i.e. the volume dominated by the trade-off solutions) based improvement function (c.f. HypI in [1]) to aggregate the objective functions. This aggregation function is Pareto compliant: any solution that improves the aggregation function implies it will improve the current estimated Pareto set. Using the set of the initial shapes and the associated aggregated function values as data a stochastic regression model is trained with a Gaussian process (\mathcal{GP}). The benefit of using \mathcal{GP} s for regression is that they provide a posterior predictive distribution given the training data, and thus querying the surrogate model for any shape results in both a mean prediction and the uncertainty associated with the prediction. This often enables the closed form calculation of a utility function: the expected improvement in (aggregation) function value (with respect to the best function value observed so far) to be obtained by querying a solution. Therefore, a strategy for (expensively) evaluating the next solution is to select the shape that maximises the expected improvement. The newly evaluated shape is then added to the training database, and a retraining of the \mathcal{GP} model ensues. The process is repeated until the budget on the number of expensive evaluations are exhausted.

In MOBO, given a shape representation \mathbf{x} and an initial set of M shapes, we expensively evaluate all shapes for D objective functions $f_1(\mathbf{x}), \dots, f_D(\mathbf{x})$. An aggregation function $g(\mathbf{x}) \equiv g(f_1(\mathbf{x}), \dots, f_D(\mathbf{x}))$, is then used to generate the initial data set $D = \{(\mathbf{x}^m, g(\mathbf{x}^m))\}_{m=1}^M$. With this, a \mathcal{GP} model may be trained. Once trained, the predictive density from the model for a shape \mathbf{x} is: $p(\hat{g}(\mathbf{x})|D)$. Given the best evaluated shape

$\mathbf{x}^* = \arg \max_{\mathbf{x}^m \in D} g(\mathbf{x}^m)$, the expected improvement of an arbitrary feasible shape \mathbf{x} is defined as:

$$\alpha(\mathbf{x}, \mathbf{x}^*) = \int_{-\infty}^{\infty} \max(\hat{g}(\mathbf{x}) - g(\mathbf{x}^*), 0) p(\hat{g}(\mathbf{x})|D) d\hat{g}(\mathbf{x}). \quad (1)$$

As the predictive distribution is Gaussian, this integral can be calculated in closed form. Thus, selecting the next shape to evaluate is the solution of the following sub-problem: $\mathbf{x}^{M+1} = \arg \max_{\mathbf{x}} \alpha(\mathbf{x}, \mathbf{x}^*)$. The training data set was augmented with the newly evaluated shape $D \leftarrow D \cup \{(\mathbf{x}^{M+1}, g(\mathbf{x}^{M+1}))\}$, and the model is retrained. In this process, when the limit on the number of expensive function evaluations is reached, the current mutually non-dominated (Pareto) set of solutions are returned. The designer (or decision maker) may then choose a design from this set.

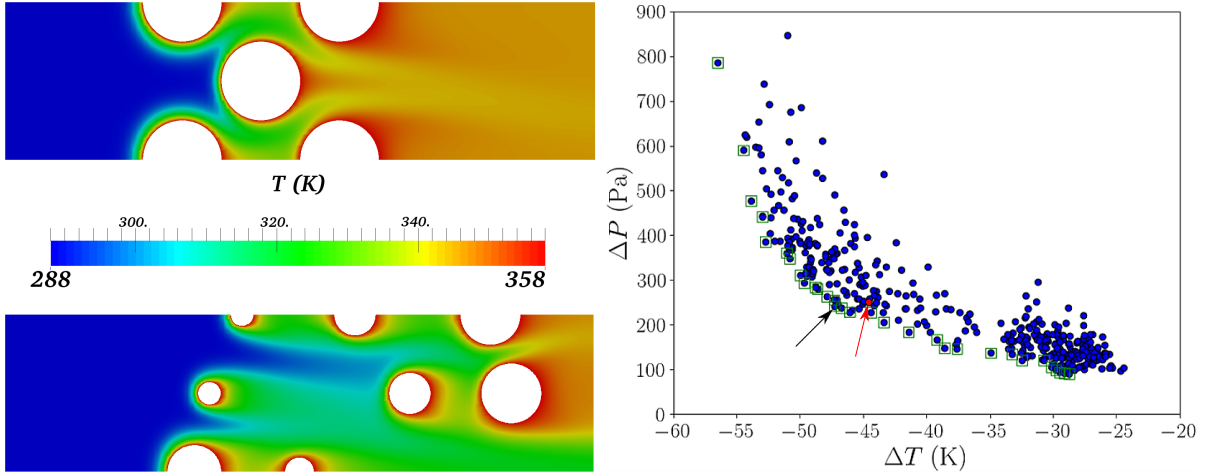


Figure 1: Left - Base geometry (top) and optimised design of the cross-flow heat exchanger (bottom). Right - Pareto front of the two objectives; the black arrow corresponds to the optimised design, the red arrow corresponds to the base design, and the green squares indicate the Pareto front.

As a brief demonstration of the proposed framework and use of MOBO, preliminary results are presented here on a cross-flow tube-bundle heat exchanger. The positions, number of, and diameters of the cross-flow tubes in the domain were chosen to be optimised. MOBO was conducted minimising the pressure and heat transfer across the domain. Figure 1 shows the resulting Pareto front of the two objectives. A number of better heat exchanger designs were achieved (relative to the base case) within 100 CFD simulations; one of these cases (indicated by the black arrow) is shown in Figure 1(left, bottom). It should be noted that for a more realistic industrial application, constraints would be applied to tube positions and diameters for manufacturability. To allow for a comprehensive investigation of the efficacy of the proposed framework and the performance of MOBO in shape optimisation, we plan to present a number of test problems similar to those commonly observed in industry, such as a turbine draft tube and the aforementioned heat exchanger.

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References

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